

Phase diagrams and critical behavior of the quantum spin-1/2 XXZ model on diamond-type hierarchical lattices

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Abstract

In this paper, the phase diagrams and the critical behavior of the spin-1/2 anisotropic XXZ ferromagnetic model (the anisotropic parameter $\Delta \in (-\infty, 1]$) on two kinds of diamond-type hierarchical (DH) lattices with fractal dimensions $d_f = 2.58$ and 3, respectively, are studied via the real-space renormalization group method. It is found that in the isotropic Heisenberg limit ($\Delta = 0$), there exist finite temperature phase transitions for the two kinds of DH lattices above. The systems are also investigated in the range of $-\infty < \Delta < 0$ and it is found that they exhibit XY-like fixed points. Meanwhile, the critical exponents of the above two systems are also calculated. The results show that for the lattice with $d_f = 2.58$, the value of the Ising critical exponent ν_I is the same as that of classical Ising model and the isotropic Heisenberg critical exponent ν_H is a finite value, and for the lattice with $d_f = 3$, the values of ν_I and ν_H agree well with those obtained on the simple cubic lattice. We also discuss the quantum fluctuation at all temperatures and find the fluctuation of XY-like model is stronger than the anisotropic Heisenberg model at the low-temperature region. By analyzing the fluctuation, we conclude that there will be remarkable effect of neglecting terms on the final results of the XY-like model. However, we can obtain approximate result at bigger temperatures and give qualitatively correct picture of the phase diagram.

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I. INTRODUCTION

The spin-1/2 anisotropic Heisenberg model, or the XXZ model, is one of the most important quantum spin models, which can be used to explain the quantum essence of many magnetic materials, such as La_2CuO_4 and thin films of ^3He [1]. Recently, for this model, many works have been done on translational symmetric lattices[2–8]. For example, F C Alcaraz and A L Malvezzi studied the XXZ chain in the presence of an external field and obtained the phase diagram of this system accurately[3]. Continentino and Sousa, respectively, have investigated the critical properties of the two-dimensional (2D) anisotropic Heisenberg model[4–6], and found that, in the isotropic Heisenberg limit, this system does not exhibit finite temperature phase transition (i.e., the critical temperature $T_C = 0$), which is in accordance with the theorem of Mermin and Wagner[9]. However, as to this model on the simple cubic lattice T_C no longer equals zero in the isotropic Heisenberg limit, which means the existence of finite temperature phase transition[7, 8, 10–12].

On the other hand, there has been some interest in the critical phenomena of XXZ model on fractal lattices, and particularly on the diamond-type hierarchical (DH) lattices. Because of the special geometrical and topological property, DH lattices are good candidates to investigate the spin systems in non-integer dimensions, and since they have a much lower symmetry than other fractals, so they may provide insights into other low-symmetry problems such as random magnets, surfaces, and the like[13, 24]. In these aspects, some theoretical works have been done. In 1983, using the renormalization group (RG) method, Caride *et al* have investigated the critical behavior of the Heisenberg model on the Wheatstone-bridge-basis hierarchical lattice. Their results show that in the isotropic Heisenberg limit T_C approaches zero as a continuous function of the anisotropic parameter[14]. Latterly, the phase diagram of this model was obtained by Souza on another kind of DH lattice with fractal dimension $d_f = 2$ [15], and the results agree well with those on the square lattice. Recently, using a real-space RG method, the anisotropic Heisenberg spin-glass model on a three-dimensional DH lattice has been studied[16].

In the study of the anisotropic Heisenberg model, many effective approximate methods have been applied. Such as the mean-field approximation[10], series expansion[12], RG method [2, 4, 7] and Monte Carlo simulation[17, 18], etc. Among these methods, the RG theory has been proved to be very powerful and it has been widely used to investigate the

critical behavior of different spin systems[2, 7, 19, 20].

In this paper, using the RG method, we investigate the quantum spin-1/2 XXZ ferromagnetic model on two kinds of DH lattices with fractal dimensions $d_f = 2.58$ and $d_f = 3$, respectively. Our results show that the systems exhibit finite temperature phase transitions in the isotropic Heisenberg limit ($\Delta = 0$). Besides, we also investigate the above systems in the range of $-\infty < \Delta < 0$ and find that they exhibit XY-like fixed points.

The outline of the remainder of this paper is as follows. In the next Section, the model and the calculation method are presented; Sec. III gives the results; Sec. IV is a discussion about some interesting quantum effects and Sec. V gives a brief conclusion. Some of the more tedious of the formulations in Sec. II are illustrated in the Appendix.

II. MODEL AND CALCULATION METHOD

The effective Hamiltonian of the XXZ model can be written as

$$H = K \sum_{\langle i,j \rangle} [(1 - \Delta) (\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y) + \sigma_i^z \sigma_j^z], \quad (1)$$

where $K = J/k_B T$, in which J is the exchange coupling parameter ($J > 0$ and $J < 0$ correspond to the ferromagnetic and the antiferromagnetic model, respectively), k_B is the Boltzmann constant, and T is the absolute temperature. σ_i^α ($\alpha = x, y, z$) are spin Pauli operators on the site i . The sum is over all the nearest-neighbor spin pairs $\langle i, j \rangle$, and $\Delta \in (-\infty, 1]$ represents the anisotropic parameter. Note that the Hamiltonian contains, as particular cases, the Ising model (for $\Delta = 1$), the isotropic Heisenberg model (for $\Delta = 0$) and the XY model (for $\Delta = -\infty$).

The DH lattices are all constructed by an iterative manner. Fig. 1(a) illustrates the first three construction stages of DH lattice with fractal dimension $d_f = 2.58$ (lattice A, for simplicity). As can be seen, the initiator is a two-point lattice joined by a single bond (construction stage $n = 0$). Then the initiator is replaced with the generator (the cluster of $n = 1$ stage). Replacing every single bond on the generator itself, we get the second stage of the lattice. If this procedure is repeated infinite times, we then construct a DH lattice with self-similar structure[21–24]. Using the same procedure as that of lattice A, we can construct another kind of DH lattice (lattice B, for simplicity) with fractal dimension $d_f = 3$ (see Fig. 1(b)).

In this section, using the RG method proposed by Caride[14, 25], we give the main calculation procedure of the XXZ ferromagnetic model on lattice A. The case of lattice B can be solved in the same way.

In the next RG procedure, the Hamiltonians, except for the Ising limit ($\Delta = 1$) and the high temperature limit ($K = 0$), among the neighboring generators do not commute with each other, which leads to the impossible of decoupling the generator from the whole lattice. In order to achieve this goal, the noncommutativity among the neighboring generators were neglected. This method had been used in Refs.[14, 15, 25, 26] and the quantum effects and the approximation of this method had been detailedly discussed in Ref.[26].

Based on the above approximation, we take out the generator from lattice A to perform the RG transformation, which is shown in Fig. 2. As can be seen, after summation of the internal spins σ_3 , σ_4 and σ_5 (decimation), the generator (Fig. 2(a)) is transformed into a new structure, which contains two spins (i.e., σ_1 and σ_2) joined by a single bond (Fig. 2(b)). This procedure can be described as

$$\text{Tr}_{3,4,5} \exp(H_{13452}) = \exp(H'_{12}), \quad (2)$$

where H_{13452} and H'_{12} are, respectively, the Hamiltonians associated with the clusters (a) and (b) in Fig. 2, $\text{Tr}_{3,4,5}$ denotes the partial trace over states of the internal spins σ_3, σ_4 and σ_5 . According to Eq. (1), the Hamiltonians H_{13452} and H'_{12} are

$$\begin{aligned} H_{13452} = & K(1 - \Delta) [(\sigma_1^x \sigma_3^x + \sigma_1^y \sigma_3^y) + (\sigma_1^x \sigma_4^x + \sigma_1^y \sigma_4^y) + (\sigma_1^x \sigma_5^x + \sigma_1^y \sigma_5^y) \\ & + (\sigma_3^x \sigma_2^x + \sigma_3^y \sigma_2^y) + (\sigma_4^x \sigma_2^x + \sigma_4^y \sigma_2^y) + (\sigma_5^x \sigma_2^x + \sigma_5^y \sigma_2^y)] \\ & + K(\sigma_1^z \sigma_3^z + \sigma_1^z \sigma_4^z + \sigma_1^z \sigma_5^z + \sigma_3^z \sigma_2^z + \sigma_4^z \sigma_2^z + \sigma_5^z \sigma_2^z) \end{aligned} \quad (3)$$

and

$$H'_{12} = K'[(1 - \Delta')(\sigma_1^x \sigma_2^x + \sigma_1^y \sigma_2^y) + \sigma_1^z \sigma_2^z] + K_0, \quad (4)$$

respectively, where K_0 is a constant included to make Eq. (2) possible.

By calculating the partial trace in Eq. (2), we can obtain the RG recurrent relations between the new parameters (K', Δ') and the original parameters (K, Δ). Firstly, we expand $\exp(H'_{12})$ as

$$\exp(H'_{12}) = a' + b'_{12}(\sigma_1^x \sigma_2^x + \sigma_1^y \sigma_2^y) + c'_{12} \sigma_1^z \sigma_2^z. \quad (5)$$

Note that, in the expansion of $\exp(H'_{12})$, the anticommutation among the spin Pauli operators are considered. Further, in the basis which simultaneously diagonalize σ_1^z and σ_2^z , we express both sides of Eq. (5) in the form of matrix. The left-hand side of Eq. (5) can be expressed as

$$\exp(H'_{12}) = \begin{pmatrix} e^{\lambda'_1} & 0 & 0 & 0 \\ 0 & \frac{1}{2}(e^{\lambda'_2} + e^{\lambda'_3}) & \frac{1}{2}(e^{\lambda'_2} - e^{\lambda'_3}) & 0 \\ 0 & \frac{1}{2}(e^{\lambda'_2} - e^{\lambda'_3}) & \frac{1}{2}(e^{\lambda'_2} + e^{\lambda'_3}) & 0 \\ 0 & 0 & 0 & e^{\lambda'_4} \end{pmatrix}, \quad (6)$$

in which

$$\lambda'_1 = \lambda'_4 = K' + K_0, \quad (7)$$

$$\lambda'_2 = -K' + 2W' + K_0 \quad (8)$$

and

$$\lambda'_3 = -K' - 2W' + K_0 \quad (9)$$

are eigenvalues of H'_{12} , where

$$W' = K'(1 - \Delta'). \quad (10)$$

Following the same steps as above, the right-hand side of Eq. (5) can also be expressed in the form

$$\begin{pmatrix} a' + c'_{12} & 0 & 0 & 0 \\ 0 & a' - c'_{12} & 2b'_{12} & 0 \\ 0 & 2b'_{12} & a' - c'_{12} & 0 \\ 0 & 0 & 0 & a' + c'_{12} \end{pmatrix}. \quad (11)$$

By combining Eqs. (6)-(11), we get

$$a' + c'_{12} = \exp(K' + K_0), \quad (12)$$

$$a' - c'_{12} = \frac{1}{2}(\exp(K' - 2K'\Delta' + K_0) + \exp(-3K' + 2K'\Delta' + K_0)) \quad (13)$$

and

$$b'_{12} = \frac{1}{4}(\exp(K' - 2K'\Delta' + K_0) - \exp(-3K' + 2K'\Delta' + K_0)). \quad (14)$$

Obviously, the coefficients a' , b'_{12} and c'_{12} are all functions of K' and Δ' .

So from Eqs. (12)-(14), we obtain the relations between the new parameters (K', Δ') and the expansion coefficients (a', b'_{12}, c'_{12}) as follows

$$\exp(4K') = \frac{(a' + c'_{12})^2}{(a' - c'_{12})^2 - 4b'^2_{12}}, \quad (15)$$

$$\exp(4K'\Delta') = \frac{(a' + c'_{12})^2}{(a' - c'_{12} + 2b'_{12})^2}. \quad (16)$$

Analogously, $\exp(H_{13452})$ can also be written as

$$\begin{aligned} \exp(H_{13452}) &= a \\ &+ \sum_{\langle i,j(>i) \rangle} [b_{ij} (\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y) + c_{ij} \sigma_i^z \sigma_j^z] \\ &+ \sum_{\langle i,j(>i) \rangle \neq \langle k,l(>k) \rangle} [d_{ij,kl} (\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y) \sigma_k^z \sigma_l^z + e_{ij,kl} (\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y) (\sigma_k^x \sigma_l^x + \sigma_k^y \sigma_l^y)] \\ &+ \sum_{\langle i,j(>i) \rangle \neq \langle k,l(>k) \rangle} f_{ij,kl} \sigma_i^z \sigma_j^z \sigma_k^z \sigma_l^z, \end{aligned} \quad (17)$$

where a , b_{ij} , c_{ij} , $d_{ij,kl}$, $e_{ij,kl}$ and $f_{ij,kl}$ are all functions of K and Δ , which can be determined by diagonalizing both sides of Eq. (17) in the same basis of σ_1^z , σ_2^z , σ_3^z , σ_4^z and σ_5^z . Because the matrices of the two sides are too lengthy, we just give the diagonal matrix form of H_{13452} in the Appendix.

From Eqs. (2), (5) and (17), we can obtain the relations among the expansion coefficients

$$a' = 8a, \quad (18)$$

$$b'_{12} = 8b_{12} \quad (19)$$

and

$$c'_{12} = 8c_{12}. \quad (20)$$

These expressions, together with Eqs. (15) and (16), we finally get

$$\exp(4K') = \frac{(a + c_{12})^2}{(a - c_{12})^2 - 4b_{12}^2}, \quad (21)$$

$$\exp(4K'\Delta') = \frac{(a + c_{12})^2}{(a - c_{12} + 2b_{12})^2}. \quad (22)$$

Since a , b_{12} and c_{12} are all functions of K and Δ , the RG recurrent relations between the new parameters (K', Δ') and the original parameters (K, Δ) are determined by Eqs. (21) and (22). However, the analytical expression about their right-hand sides are difficult to obtain. In order to obtain the phase diagram and the fixed points, we will numerically solve the above two equations and the results will be presented in the next section.

III. RESULTS

By numerically iteration, the RG recurrent equations (21) and (22), the phase diagram and the fixed points for the system with fractal dimension $d_f = 2.58$ can be obtained, which are shown in Fig. 3. The curve (a) in Fig. 3 gives the critical line of the system. As can be seen, in the range of $\Delta \in [0, 1]$, the phase space is divided into the paramagnetic phase (P) and the ferromagnetic phase (F) by the critical line. In this range, we can also find that the system exhibits two unstable fixed points, i.e., the Ising unstable fixed point (IP for short) $(\Delta, 1/K) = (1, 2.77)$ and the isotropic Heisenberg unstable fixed point (HP) $(0, 1.55)$. In fact, the value of the IP is in accordance with that of the classical model[21, 22]. At the IP, the correlation length critical exponent can be calculated by

$$\nu_I = \frac{\ln b}{\ln \lambda}, \quad (23)$$

in which, $b = 2$ is the scaling factor and $\lambda = (\partial K'/\partial K)_{\Delta=1, K=0.36} = 1.86$, thus, $\nu_I = 1.12$. We note that this value is the same as that of the classical Ising model[21–23]. It is worth mentioning that, at the HP, the system exhibits a finite temperature phase transition with critical temperature $T_C = 1/K_C = 1.55$. However, this is disagree with the result of the Wheatstone-bridge-basis hierarchical lattice[14], where only zero temperature phase transition exists, i.e., $T_C = 0$ when $\Delta = 0$ (curve (b) in Fig. 3). In addition, the isotropic Heisenberg critical exponent is obtained as $\nu_H = 2.04$ which differs greatly from the results ($\nu_H = \infty$) of the 2D regular lattices[7, 8] and other hierarchical lattices with lower fractal dimensions ($d_f < 2.58$)[14, 15].

We also investigate the above system in the range of $-\infty < \Delta < 0$. Our results show that the system exhibits an unstable fixed point, which is not given in Refs. [6, 14] and we call it XY-like fixed point (XYP). The critical line between the HP and the XYP divides the phase space into paramagnetic phase (P) and ferromagnetic phase (F) as well.

Using the same calculation procedure as the lattice A, we can also investigate the critical behavior of the XXZ model on the lattice B, i.e., the DH lattice with $d_f = 3$. The phase diagram and the fixed points are presented in Fig. 4. We can see that the phase space is divided into paramagnetic phase (P) and ferromagnetic phase (F) by the critical line. In the range of $\Delta \in [0, 1]$, the system also exhibits two unstable fixed points, i.e., the Ising fixed point (IP) and the isotropic Heisenberg fixed point (HP). At the IP $(\Delta, 1/K) = (1, 3.79)$ we obtain the critical temperature $T_C = 3.97$ and the critical exponent $\nu_I = 0.95$.

Compared with the results of three dimensional Heisenberg model calculated by other RG methods[26, 27], our results are more consistent with that from series expansion ($T_C = 4.54, \nu_I = 0.63$)[12]. At the HP ($\Delta, 1/K$) = (0, 2.36), the critical temperature $T_C = 2.36$ is very close to that of three-dimensional Heisenberg system ($T_C = 2.41$)[11]. In addition, the critical exponent is $\nu_H = 1.69$ which agrees well with that obtained by Sousa *et al* on the simple cubic lattice where $\nu_H = 1.64$ [28]. In summary, we can see that the lattice B can be regarded as an approximation for the simple cubic lattice. Besides, just as the case of the lattice A, the system on lattice B also exhibits a XY-like fixed point (XYP) ($\Delta, 1/K$) = (-1.99, 8.44).

IV. DISCUSSION

In this section, we discuss the possible effects of quantum fluctuation. We assume the generator of lattice A as a whole. In this case, there will be no noncommutativity and the result should be exact in our calculation. With this method, the exact calculation of the DH lattice will be noted $[K'(K, \Delta), \Delta'(K, \Delta)]$. On the other hand, for the RG transformation in Fig. 2, we apply a modified Migdal-Kadanoff method, which is an approximate one. In this method, the original cell (Fig. 2(a)) can be considered as a combination of 3 arrays in parallel, each of which is made up of two interactions in series. The renormalized interaction K and anisotropy Δ can be firstly calculated for each combination in series and then combined in parallel. The approximate calculation provides $[3K''(K, \Delta), \Delta''(K, \Delta)]$. We use the convenient ratios introduced in Ref. [25]

$$R^K = \frac{3K''(K, \Delta; K, \Delta)}{K'(K, \Delta)} \quad (24)$$

and

$$R^\Delta = \frac{\Delta''(K, \Delta; K, \Delta)}{\Delta'(K, \Delta)} \quad (25)$$

The T -dependences of R^K and R^Δ for typical values of Δ are indicated in Fig. 5. In the high temperature limit, both R^K and R^Δ tend to unity for all values of Δ ($0 \leq \Delta \leq 1$ and $\Delta < 0$). In the range of low temperature, where the quantum effect tends to drive the system to a disordered phase, both R^K and R^Δ show oscillational behaviours. The fact is usually due to quantum fluctuation which, at low temperatures (T) and smaller anisotropy (Δ) are important[16]. As we see in Fig. 5, the quantum fluctuation of XY-like model ($\Delta < 0$)

is stronger than the anisotropic Heisenberg model ($0 \leq \Delta \leq 1$) at the low-temperature region. So, there will be considerable error when we calculate the XY-like model at lower temperatures. However, in the range of $0 \leq \Delta \leq 1$, it is a very good approximation and when the anisotropy Δ is negative, as we can see in Fig. 5, it follows the same tendency as the positive one. So, we can obtain approximate result at bigger temperatures and give qualitatively correct picture of the phase diagram. When it comes to the lattice B, both R^K and R^Δ have the same type of behaviour and we can obtain the same conclusion.

V. CONCLUSION

In conclusion, using the RG method, we have studied the quantum spin-1/2 anisotropic XXZ model on two kinds of DH lattices with fractal dimensions $d_f = 2.58$ and 3, respectively. Phase diagrams, fixed points and critical exponents of the systems are obtained. The results show that, in the Ising limit ($\Delta = 1$), the values of the fixed points and the critical exponents agree well with those in Refs. [12, 22, 23]. In the isotropic Heisenberg limit ($\Delta = 0$), there are finite temperature phase transitions on the above two lattices. Furthermore, the systems exhibit XY-like fixed points in the range of $-\infty < \Delta < 0$. The quantum effects of this system show that, at low temperatures, the XY-like model has stronger fluctuation than the anisotropic Heisenberg model. So, we conclude that there will be a considerable error when we calculate the XY-like model at low temperature. Besides, our results also indicate that the DH lattice with $d_f = 3$ can be regarded as an approximation for the simple cubic lattice. As a comment, this method can be extended to investigate spin systems with $S > 1/2$ on other lattices and we are presently working along these lines.

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Appendix

In the basis of $\sigma_1^z, \sigma_2^z, \sigma_3^z, \sigma_4^z$ and σ_5^z , H_{13452} can be expressed as a 32×32 matrix in the form of

$$H_{13452} = \begin{pmatrix} A & 0 & 0 & 0 & 0 & 0 \\ 0 & B & 0 & 0 & 0 & 0 \\ 0 & 0 & C & 0 & 0 & 0 \\ 0 & 0 & 0 & C & 0 & 0 \\ 0 & 0 & 0 & 0 & B & 0 \\ 0 & 0 & 0 & 0 & 0 & A \end{pmatrix},$$

in which $A = 6K$,

$$B = \begin{pmatrix} 0 & 0 & 2W & 2W & 2W \\ 0 & 0 & 2W & 2W & 2W \\ 2W & 2W & 2K & 0 & 0 \\ 2W & 2W & 0 & 2K & 0 \\ 2W & 2W & 0 & 0 & 2K \end{pmatrix},$$

$$C = \begin{pmatrix} -6K & 2W & 2W & 2W & 2W & 2W & 2W & 0 & 0 & 0 \\ 2W & 0 & 0 & 0 & 0 & 0 & 0 & 2W & 2W & 0 \\ 2W & 0 & 0 & 0 & 0 & 0 & 0 & 2W & 0 & 2W \\ 2W & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2W & 2W \\ 2W & 0 & 0 & 0 & 0 & 0 & 0 & 2W & 2W & 0 \\ 2W & 0 & 0 & 0 & 0 & 0 & 0 & 2W & 0 & 2W \\ 2W & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2W & 2W \\ 0 & 2W & 2W & 0 & 2W & 2W & 0 & -2K & 0 & 0 \\ 0 & 2W & 0 & 2W & 2W & 0 & 2W & 0 & -2K & 0 \\ 0 & 0 & 2W & 2W & 0 & 2W & 2W & 0 & 0 & -2K \end{pmatrix},$$

where $W = K(1 - \Delta)$.

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Figure Captions

Fig. 1 The first two construction stages of the DH lattices. (a) the DH lattice with fractal dimension $d_f = 2.58$, (b) the DH lattice with $d_f = 3$.

Fig. 2 The procedure of the RG transformation. After a step of the RG transformation the generator (a) is transformed into a bond (b).

Fig. 3 Phase diagram of the DH lattice with $d_f = 2.58$. The critical line (a) separates the phase space into paramagnetic phase (P) and ferromagnetic phase (F). The IP, HP and XYP, respectively, denote the Ising, isotropic Heisenberg and XY fixed points. (b) is the critical line of the Wheatstone-bridge-basis hierarchical lattice for comparison.

Fig. 4 Phase diagram of the DH lattice with $d_f = 3$. The IP, HP and XYP, respectively, denote the Ising, isotropic Heisenberg and XY fixed points. P and F correspond to the paramagnetic phase and ferromagnetic phase, respectively.

Fig. 5 Thermal dependence of the ratios R^K and R^Δ respectively defined by Eqs. (24) and (25), for typical values of Δ .

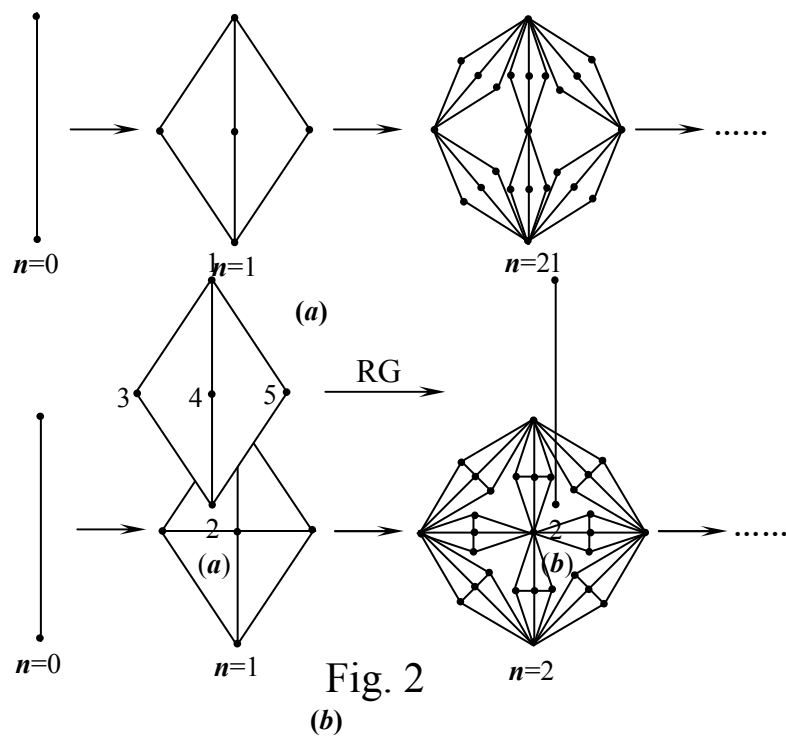


Fig. 2

Fig. 1

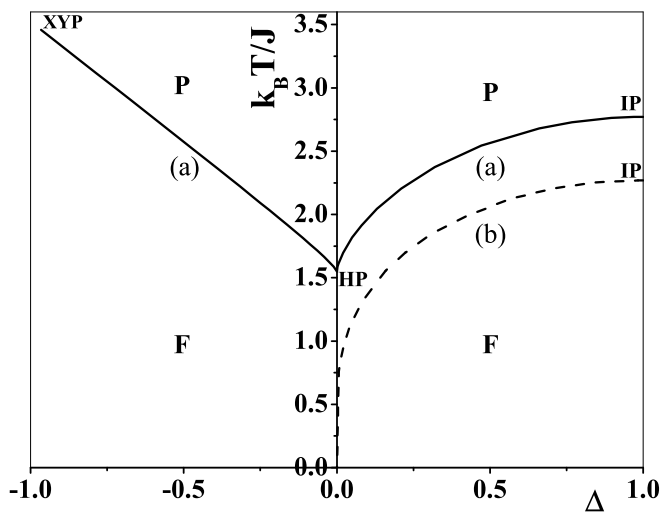


Fig.3

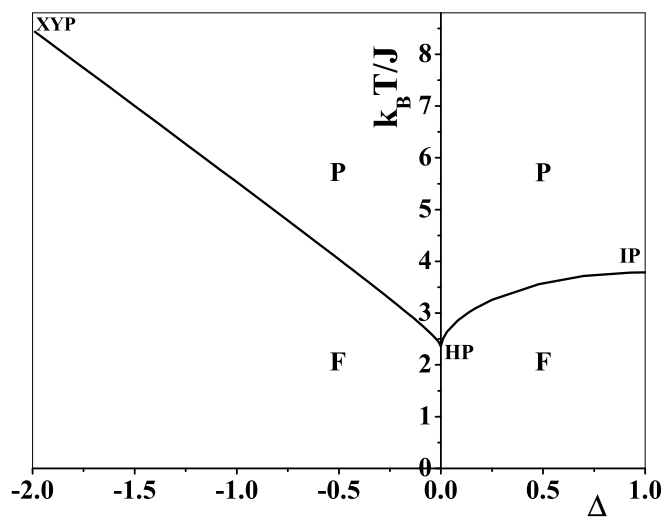


Fig. 4

